MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **61** (2009) 643-651

ISSN 0340 - 6253

Wiener and Schultz Molecular Topological Indices of Graphs with Specified Cut Edges *

Hongbo Hua†

Department of Computing Science, Huaiyin Institute of Technology, Huaian, Jiangsu 223000, People's Republic of China

(Received January 30, 2008)

Abstract

Let G be a simple, undirected and connected graph. The Wiener index $W(G)$ of G is defined to be the sum of distances between all pair of vertices of G, that is, $W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(i,j)$. The Schultz molecular topological index of G, denoted by $MTI(G)$, is defined to be the summation $\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(i)\left(A_{ij} + d_G(i,j)\right)$, where n is the order of G, $d_G(i)$ is the degree of vertex i in G, and $d_G(i,j)$ is the distance between vertices i and j and A_{ij} is the $(i,j)-th$ entry of the adjacency matrix A of G. Denote by $\mathcal{G}_{n,k}$ the set of graphs with n vertices and k cut edges. In this note, we determine resp. the minimal elements with respect to $W(G)$ and $MTI(G)$ among all elements G in $\mathcal{G}_{n,k}(1 \le k \le n-3)$.

1 Introduction

Given that G is a simple, undirected and connected graph with $V(G)$ and $E(G)$ being the set of vertices and edges, respectively. For any two vertices i and j in G, we mean, by $d_G(i)$, the degree of vertex i, the number of edges incident with i in G, while, by $d_G(i,j)$, the distance between i and j in G, the length of the shortest path connecting i and j in G.

*Partially supported by SRFs of Huaiyin Institute of Technology (HGQ0611, HGQN0726, HGQN0727).

†Email address: hongbo.hua@gmail.com

The Schultz molecular topological index, or simply denoted as MTI, of a (chemical) graph G proposed by Schultz [1] in 1989 is defined as

$$MTI = MTI(G) = \sum_{i=1}^{n}\sum_{j=1}^{n} d_G(i)\left(A_{ij} + d_G(i,j)\right),$$

where n is the order of G, the number of vertices in G, $d = (d_G(1), d_G(2), \cdots, d_G(n))$ is the degree sequence in G, and A_{ij} is the $(i,j) - th$ entry of the adjacency matrix A of G.

Let $D_G(i) = \sum_{j=1}^{n} d_G(i,j)$ be the sum of distances between the vertex i and all the remaining vertices in G. The Schultz molecular topological index can also be expressed via the following manner [3]:

$$MTI = MTI(G) = \sum_{i=1}^{n} d_G^2(i) + \sum_{i=1}^{n} d_G(i)D_G(i),$$

which can be further reduced to the following form:

$$MTI = MTI(G) = \sum_{i=1}^{n} d_G^2(i) + \sum_{i,j=1}^{n} (d_G(i) + d_G(j))d_G(i,j). \qquad (1)$$

Another much–studied distance–based molecular topological index is the Wiener index $W(G)$, for this index see the recent survey [8,9], which is defined to be the sum of distances between all pair of vertices of G, that is,

$$W = W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(i,j).$$

It has been demonstrated that MTI and W are closely mutually related for certain amount of molecular graphs [2,3,5–9]. Moreover, it has been proved [5,7] that the Schultz molecular topological index has the same discriminating power with the Wiener index

$$MTI(G_1) = MTI(G_2) \quad \text{if and only if} \quad W(G_1) = W(G_2) \qquad (2)$$

for arbitrary catacondensed benzenoid graphs. So it is both significant and interesting to study the Schultz molecular topological index for some given class of graphs, no matter whether they are molecular graphs or not.

Most recent research papers concerning on Schultz molecular topological index are mainly restricted to give formulas for computing the exact value of MTI for some molecular graphs, see for instance [10–12]. In general, for any given graph G, its Schultz molecular topological index $MTI(G)$ is not always easily calculated. So it makes sense to determine the (upper and/or lower) bound(s) of $MTI(G)$ among a given class of graphs, or, to characterize the graphs with extremal (maximal or/and minimal) Schultz molecular topological index among a certain class of graphs. Based on such a consideration, we shall determine resp. in this work that the graphs with minimal Schultz molecular topological index and Wiener index among all elements in $\mathcal{G}_{n,k}$, the set of graphs with n vertices and k cut edges.

2 Graph in $\mathcal{G}_{n,k}$ with minimal value of $MTI(G)$ or $W(G)$

As usual, we begin with some notations and terminology. For any two graphs G_1 and G_2, if there exists a bridge uv between G_1 and G_2 such that $u \in G_1$ and $v \in G_2$, we denote this graph as G_1uvG_2. If there are a sequence of graphs $G_1, G_2, \cdots, G_s (s \geq 2)$ with all graphs sharing one common (cut) vertex x, then we denote this graph as $G_1xG_2 \cdots xG_s$.

Denote by $\mathcal{G}_{n,k}$ the set of graphs with n vertices and k cut edges. For a $n-$vertex connected graph G having no cycle, namely, a tree on n vertices, we know that G has exactly $n-1$ cut edges and the tree with minimal $MTI(G)$ can be easily determined by using Eq.(2), since star S_n has the minimum cardinality of $W(G)$, which has been determined long time ago. For a connected graph G on n vertices having at least one cycle, the number of its cut edges is at most $n-3$. So it will be always assumed in the subsequent part of this paper that G has k cut edges with $1 \leq k \leq n-3$.

Operation A

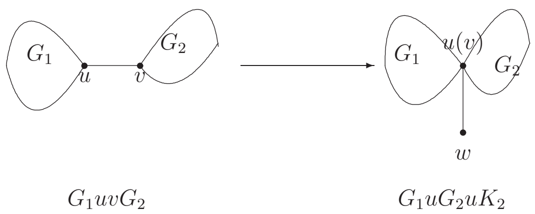


Fig. 1.

In the following, we shall introduce some lemmas which are crucial to the proofs of our main results. Let $|V(G)|$ denote the number of vertices in G, then we have

Lemma 1. *Let G_1uvG_2 and $G_1uG_2uK_2$ be two graphs with $|V(G_1)|, |V(G_2)| \geq 2$, as shown in Fig.1. Then $MTI(G_1uvG_2) > MTI(G_1uG_2uK_2)$.*

Proof. Set $G_1^* = G_1uvG_2$, $G_2^* = G_1uG_2uK_2$. By Eq. (1), we obtain

$MTI(G_1uG_2uK_2) - MTI(G_1uvG_2)$

$$= (d_{G_1^*}(u) + d_{G_1^*}(v) - 1)^2 + 1^2 - d^2_{G_1^*}(u) - d^2_{G_1^*}(v) + \sum_{x\in G_1-\{u\}} (1 + d_{G_2^*}(x))d_{G_2^*}(w,x) + \sum_{y\in G_2-\{v\}} (1 + d_{G_2^*}(y))d_{G_2^*}(w,y) - \sum_{x\in G_1-\{u\}} (d_{G_1^*}(v) + d_{G_1^*}(x))d_{G_1^*}(v,x) - \sum_{y\in G_2-\{v\}} (d_{G_1^*}(u) + d_{G_1^*}(y))d_{G_1^*}(u,y) + (d_{G_2^*}(u) + d_{G_2^*}(w)) \times 1 - (d_{G_1^*}(u) + d_{G_1^*}(v)) \times 1 + \sum_{x\in G_1-\{u\}} (d_{G_2^*}(u) + d_{G_2^*}(x))d_{G_2^*}(u,x) + \sum_{y\in G_2-\{v\}} (d_{G_2^*}(v) + d_{G_2^*}(y))d_{G_2^*}(v,y) - \sum_{x\in G_1-\{u\}} (d_{G_1^*}(u) + d_{G_1^*}(x))d_{G_1^*}(u,x) - \sum_{y\in G_2-\{v\}} (d_{G_1^*}(v) + d_{G_1^*}(y))d_{G_1^*}(v,y) + \sum_{x\in G_1-\{u\}} \sum_{y\in G_2-\{v\}} (d_{G_2^*}(x) + d_{G_2^*}(y))d_{G_2^*}(x,y) - \sum_{x\in G_1-\{u\}} \sum_{y\in G_2-\{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x,y).$$

For $x \in G_1 - \{u\}$, $y \in G_2 - \{v\}$, we clearly have $d_{G_2^*}(x) = d_{G_1^*}(x)$, $d_{G_2^*}(y) = d_{G_1^*}(y)$, $d_{G_2^*}(u,x) = d_{G_1^*}(u,x)$, $d_{G_2^*}(v,y) = d_{G_1^*}(v,y)$, and $d_{G_2^*}(x,y) = d_{G_1^*}(x,y) - 1$. Also, $d_{G_2^*}(w,x) = d_{G_1^*}(v,x)$, $d_{G_2^*}(w,y) = d_{G_1^*}(u,y)$.

So we have

$MTI(G_1uG_2uK_2) - MTI(G_1uvG_2)$

$$\begin{aligned} &= 2(d_{G_1^*}(u) - 1)(d_{G_1^*}(v) - 1) + \sum_{x\in G_1-\{u\}} (1 - d_{G_1^*}(v))d_{G_1^*}(v,x) + \sum_{y\in G_2-\{v\}} (1 - d_{G_1^*}(u))d_{G_1^*}(u,y) + \sum_{x\in G_1-\{u\}} (d_{G_1^*}(v) - 1)d_{G_1^*}(u,x) + \\ &\quad \sum_{y\in G_2-\{v\}} (d_{G_1^*}(u) - 1)d_{G_1^*}(v,y) - \sum_{x\in G_1-\{u\}} \sum_{y\in G_2-\{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x,y) \\ &\leq 2(d_{G_1^*}(u) - 1)(d_{G_1^*}(v) - 1) + \sum_{x\in G_1-\{u\}} (1 - d_{G_1^*}(v))d_{G_1^*}(u,x) + \sum_{y\in G_2-\{v\}} (1 - d_{G_1^*}(u))d_{G_1^*}(v,y) + \sum_{x\in G_1-\{u\}} (d_{G_1^*}(v) - 1)d_{G_1^*}(u,x) + \\ &\quad \sum_{y\in G_2-\{v\}} (d_{G_1^*}(u) - 1)d_{G_1^*}(v,y) - \sum_{x\in G_1-\{u\}, y\in G_2-\{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x,y) \\ &= 2(d_{G_1^*}(u) - 1)(d_{G_1^*}(v) - 1) - \sum_{x\in G_1-\{u\}} \sum_{y\in G_2-\{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x,y). \end{aligned}$$

Note that $d_{G_1^*}(x,y) \geq 3$, $d_{G_1^*}(x) + d_{G_1^*}(y) \geq 2$. So we have

$$\begin{aligned} \sum_{x\in G_1-\{u\}} \sum_{y\in G_2-\{v\}} (d_{G_1^*}(x) + d_{G_1^*}(y))d_{G_1^*}(x,y) &\geq 6 \sum_{x\in G_1-\{u\}} 1 \sum_{y\in G_2-\{v\}} 1 \\ &= 6(|V(G_1)| - 1)(|V(G_2)| - 1). \end{aligned}$$

But $2(d_{G_1^*}(u)-1)(d_{G_1^*}(v)-1) \leq 2(|V(G_1)|-1)(|V(G_2)|-1)$, which concludes the proof. ■

Similar to Lemma 1, we can obtain:

Lemma 2. *Let G_1uvG_2 and $G_1uG_2uK_2$ be two graphs with $|V(G_1)|, |V(G_2)| \geq 2$, as shown in Fig.1. Then $W(G_1uvG_2) > W(G_1uG_2uK_2)$.*

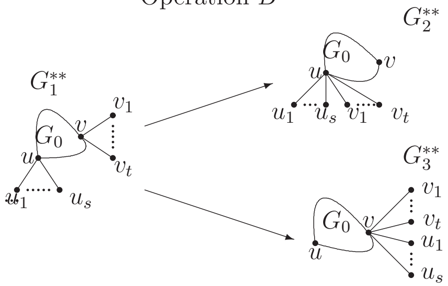


Fig. 2.

Lemma 3. *Let G_1^{**}, G_2^{**} and G_3^{**} be graphs with $|V(G_0)| \geq 3$, as shown in Fig.2. Then $MTI(G_1^{**}) > MTI(G_2^{**})$ or $MTI(G_1^{**}) > MTI(G_3^{**})$.*

Proof. Write $G_0^* = G_0 - \{u, v\}$. By Eq. (1), we obtain

$$\begin{aligned}
& MTI(G_2^{**}) - MTI(G_1^{**}) \\
= \; & (d_{G_0}(u)+s+t)^2 + d_{G_0}^2(v) - (d_{G_0}(u)+s)^2 - (d_{G_0}(v)+t)^2 + \\
& \sum_{w\in G_0^*} [(t+d_{G_0}(u)+s)+d_{G_0}(w)]\, d_{G_0}(u,w) - \sum_{w\in G_0^*} [(s+d_{G_0}(u))+d_{G_0}(w)]\, d_{G_0}(u,w) + \\
& \sum_{w\in G_0^*} (d_{G_0}(v)+d_{G_0}(w))d_{G_0}(v,w) - \sum_{w\in G_0^*} [(d_{G_0}(v)+t)+d_{G_0}(w)]d_{G_0}(v,w) + \\
& t[(s+d_{G_0}(u)+t)+1]\times 1 - t(d_{G_0}(u)+s+1)(d_{G_0}(u,v)+1) + s[(s+d_{G_0}(u)+t)+1]\times 1 - \\
& s[(s+d_{G_0}(u))+1]\times 1 + s(d_{G_0}(v)+1)(d_{G_0}(v,u)+1) - s(d_{G_0}(v)+t+1)(d_{G_0}(v,u)+1) + \\
& st(1+1)\times 2 - st(1+1)(2+d_{G_0}(v,u)) + t\sum_{w\in G_0^*} (1+d_{G_0}(w))(d_{G_0}(u,w)+1) - \\
& t\sum_{w\in G_0^*} (1+d_{G_0}(w))(d_{G_0}(v,w)+1) + t(d_{G_0}(v)+1)(d_{G_0}(v,u)+1) - t(d_{G_0}(v)+t+1)\times 1 \\
= \; & t[\sum_{w\in G_0^*} (2+d_{G_0}(w))(d_{G_0}(u,w)-d_{G_0}(v,w)) - (d_{G_0}(u)-d_{G_0}(v)+3s)d_{G_0}(u,v) + 2s + \\
& 2d_{G_0}(u) - 2d_{G_0}(v)].
\end{aligned}$$

Similarly, we have

$MTI(G_3^{**}) - MTI(G_1^{**})$

$$= s[\sum_{w \in G_0^*} (2 + d_{G_0}(w))(d_{G_0}(v,w) - d_{G_0}(u,w)) - (d_{G_0}(v) - d_{G_0}(u) + 3t)d_{G_0}(u,v) + 2t + 2d_{G_0}(v) - 2d_{G_0}(u)].$$

If $MTI(G_1^{**}) > MTI(G_2^{**})$, the proof is completed. Otherwise, we have

$$\sum_{w \in G_0^*} (2+d_{G_0}(w))(d_{G_0}(u,w)-d_{G_0}(v,w))-(d_{G_0}(u)-d_{G_0}(v)+3s)d_{G_0}(u,v)+2s+2d_{G_0}(u)-2d_{G_0}(v) \geq 0,$$

that is, $\sum_{w \in G_0^*} (2 + d_{G_0}(w))(d_{G_0}(v,w) - d_{G_0}(u,w)) \leq -(d_{G_0}(u) - d_{G_0}(v) + 3s)d_{G_0}(u,v) + 2s + 2d_{G_0}(u) - 2d_{G_0}(v)$.

So we get

$MTI(G_3^{**}) - MTI(G_1^{**})$

$$\begin{aligned} &\leq s[-(d_{G_0}(u) - d_{G_0}(v) + 3s)d_{G_0}(u,v) + 2s + 2d_{G_0}(u) - 2d_{G_0}(v) - (d_{G_0}(v) - d_{G_0}(u) + 3t)d_{G_0}(u,v) \\ &\quad +2t + 2d_{G_0}(v) - 2d_{G_0}(u)] \\ &= s[2(s+t) - 3(s+t)d_{G_0}(u,v)] < 0, \end{aligned}$$

resulting in $MTI(G_1^{**}) > MTI(G_3^{**})$, which completes the proof. ■

By the same reasoning as used in Lemma 3, we can demonstrate:

Lemma 4. *Let G_1^{**}, G_2^{**} and G_3^{**} be graphs with $|V(G_0)| \geq 3$, as shown in Fig.2. Then $W(G_1^{**}) > W(G_2^{**})$ or $W(G_1^{**}) > W(G_3^{**})$.*

Theorem 5. *Let G be a connected simple $(n,m)-$graph, a graph with n vertices and m edges. Then $MTI(G) \geq 4(n-1)m$ with equality if and only if the diameter of G is no more than two.*

Proof. Suppose that G is a graph of diameter at least two. By definition of $MTI(G)$, we have

$$\begin{aligned} MTI(G) &= \sum_{i=1}^{n} d_G^2(i) + \sum_{i=1}^{n} d_G(i)D_G(i) \\ &\geq \sum_{i=1}^{n} d_G^2(i) + \sum_{i=1}^{n} d_G(i)\left[d_G(i) + 2(n-1-d_G(i))\right] \\ &= 4(n-1)m. \end{aligned}$$

It is not difficult to see that the equality holds in the above inequality if and only if the diameter of G is exactly two.

When the diameter of G is one, namely, $G \cong K_n$, we have $MTI(G) = 2n(n-1)^2 = 4(n-1)m$. Therefore, the proof of the present theorem is completed. ■

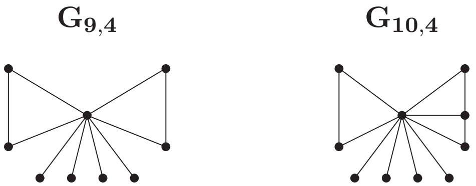


Fig. 3. Examples of graphs $G_{n,k}$ with given values of n and k

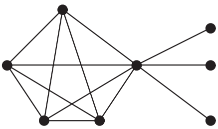
We use $G_{n,k}$ to denote the graph by introducing $\frac{n-k-1}{2}$ independent edges to the star S_n if $n-k-1$ is even and by adding $\frac{n-k-2}{2}$ independent edges to the star S_{n-1}, and then inserting a vertex to one of the above newly added independent edges and connecting it to the center of star if $n-k-1$ is odd. Then we have:

Theorem 6. *Let $G \in \mathcal{G}_{n,k}$ with $1 \leq k \leq n-3$, then $MTI(G) \geq MTI(G_{n,k})$ with equality if and only if $G \cong G_{n,k}$.*

Proof. Let G_{min} be a graph in $\mathcal{G}_{n,k}$ such that $MTI(G)$ assumes the minimum cardinality. Then all cut edges in G_{min} must be pendent edges. Moreover, all pendent vertices in G_{min} must be adjacent to one common vertex, say v. If G_{min} is not the graph as claimed above, then by Lemmas 1 and/or 3, we must get a graph G' from G_{min} by using Operation A or B such that $MTI(G') < MTI(G_{min})$, a contradiction. Then we must have $G_{min} \cong HvS_{k+1}$, where H is a $2-edge-$connected graph and S_{k+1} is a star of $k+1$ vertices. If there exists a vertex $u \in H - \{v\}$ such that u is not adjacent to v, then the diameter of G_{min} is greater than or equal to 3, which contradicts the minimality of $MTI(G_{min})$ by Theorem 5. So we have $d_{G_{min}}(v) = n-1$. By Theorem 5, in order for $MTI(G)$ to achieve the minimum cardinality, we must guarantee that m, the number of edges in G_{min}, takes the value as small as possible. Therefore we must have $G_{min} \cong G_{n,k}$, and the proof is completed. ■

Similar to Theorem 6, by means of Lemmas 2 and/or 4, we can prove with no difficulty that:

Theorem 7. *Let $G \in \mathcal{G}_{n,k}$ with $1 \leq k \leq n-3$, then $W(G) \geq W(K_{n-k}^{k})$ with equality if and only if $G \cong K_{n-k}^{k}$, the graph obtained by attaching k pendent edges to any one vertex of K_{n-k}, the complete graph on $n-k$ vertices.*



$\mathbf{K_5^3}$

Fig. 4. An example of graph K_{n-k}^{k} with $n = 8$ and $k = 3$.

It may be interesting to investigate the graph with maximal $MTI(G)/W(G)$ among all elements G in $\mathcal{G}_{n,k}$ for $1 \leq k \leq n-3$. But, as far as the author can see, it seems much more difficult than the present work we did here.

References

[1] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes *J. Chem. Inf. Comput. Sci.* 29(1989) 227-228.

[2] I. Gutman, S. Klavžar, Bounds for the Schultz molecular topological index of benzenoid systems in terms of the Wiener index, *J. Chem. Inf. Comput. Sci.* 37 (1997) 741-744.

[3] S. Klavžar, I. Gutman, A comparision of the Schultz molecular topological index with the Wiener index, *J. Chem. Inf. Comput. Sci.* 36 (1996) 1001-1003.

[4] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* 34 (1994) 1087-1089.

[5] A. A. Dobrynin, Explict relation between the Wiener index and the Schultz molecular topological index of catacondensed benzenoid graphs, *Croat. Chem. Acta* 72 (1999) 869-874.

[6] D. Plavšić, S. Nikolić, N. Trinajstić, D. J. Klein, Relation between the Wiener index and the Schultz molecular topological index for several classes of chemical graphs, *Croat. Chem. Acta* 66 (1993) 345-353.

[7] A. A. Dobrynin, Discriminating power of the Schultz index for catacondensed benzenoid graphs, *MATCH Commun. Math. Comput. Chem.* 38 (1998) 19-35.

[8] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* 66 (2001) 211-249.

[9] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* 72 (2002) 247-294.

[10] H. Deng, The Schultz molecular topological index of polyhex nanotubes, *MATCH Commun. Math. Comput. Chem.* 57 (2007) 677-684.

[11] L. Xu, H. Deng, The Schultz molecular topological index of C_4C_8 nanotubes, *MATCH Commun. Math. Comput. Chem.* 59 (2008) 421-428.

[12] S. Chen, Q. Jang, Y. Hou, The Wiener and Schultz index of nanotubes covered by C_4, *MATCH Commun. Math. Comput. Chem.* 59 (2008) 429-435.